Ill-Posed Inverse Problems: Algorithms and Applications

Total Least Squares

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Parameter Estimation Problem

- **Classical Approach** Linear Least Squares(A is exactly specified.)

$$x_{LS} = \arg\min_x ||Ax - b||_2^2$$

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- **Dense** A Form QR Decomposition of A, solve *directly* $Rx = Q^T b$.
- **Sparse** A Use *iterative* techniques, CG, Krylov subspace, etc.

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- **General Applications:** Image Processing, Signal Identification
- **Our Motivation** Seismic & Medical Signal Restoration

Invariant Model

- Signal degradation is modeled as a convolution

$$g = f \otimes h + n$$

  - where g is the blurred signal
  - f is the unknown signal
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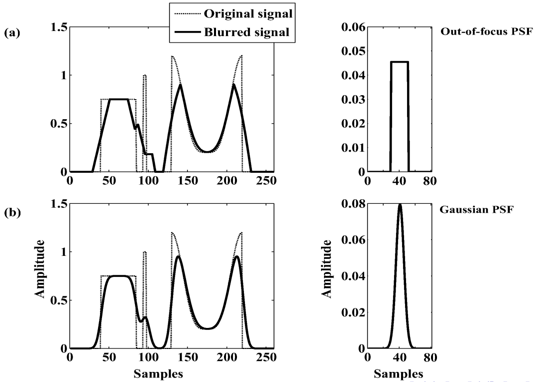
- **Matrix Formulation** H is Toeplitz (structured)

$$g = Hf + n$$

Example Of Convolution

$$g = f \otimes h + n$$



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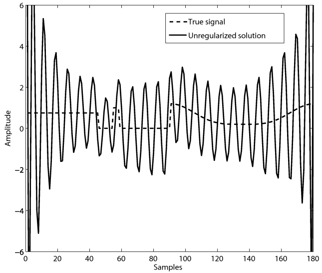
- Reconstruction with $n \in \mathbb{N}(0, 10^{-7})$



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- Regularize

$$\hat{f} = \arg\min_{f}\{\|g - f \otimes h\|_2^2 + \lambda R(f)\},$$

where $R(f)$ is the penalty term and λ is a penalty parameter.

Standard Methods

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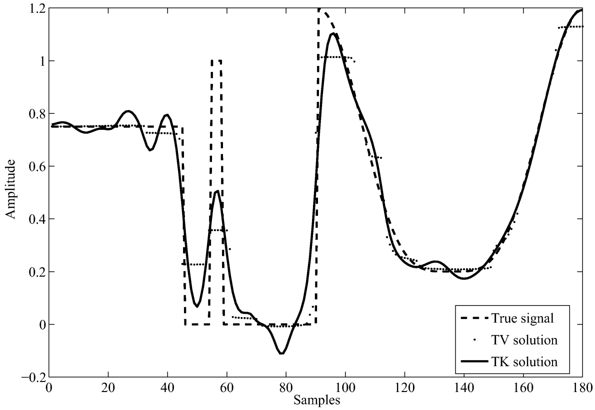
- Sparse deconvolution (L^1)

$$R(f) = \|f\|_1 = \int_\Omega |f(x)| dx.$$

Comparing TV and TK Regularization



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- TK yields a smooth reconstruction
- To find the minimum we use a limited memory BFGS method

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- **Evaluation** of the OF and its gradient **is cheap** (some FFTs and sparse matrix-vector multiplications)

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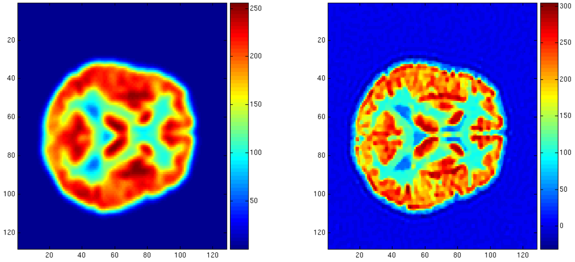

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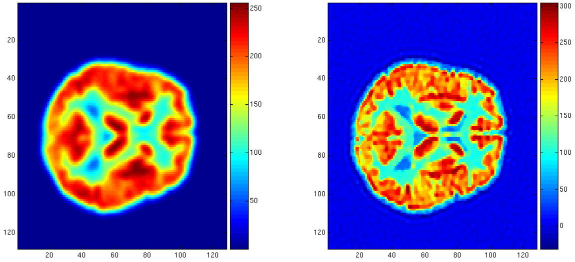
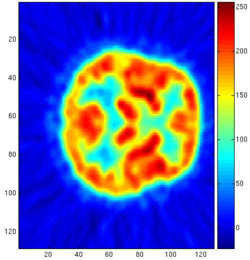
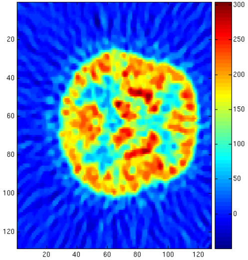


- **Note:** PSF is known regularize with TV

Real PET data





- Reconstruction done using Filtered Back Projection
- PSF estimated by a Gaussian
- TV regularization

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- Improvement requires better approximation of the PSF
- Increased Artifacts and noise. (More post processing can improve this)

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- Example: Dynamic PET Estimate parameters $\mathcal{K} = (K_1, k_2, k_3, k_4)$, which satisfy

$$y(t) = u(t) \otimes \left(c_1(\mathcal{K}) e^{-\lambda_1(\mathcal{K})t} + c_2(\mathcal{K}) e^{-\lambda_2(\mathcal{K})t} \right).$$

Nonlinear parameter estimation can be converted to linear form

$$H = [\int(u); \int\int(u); \int(y); \int\int(y)],$$

$g = Hf$, but $f = f(\mathcal{K})$, is non linear.

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- Signal Processing: Minimum norm method (Kumaresan &Tufts, 1983)

$$\min \|(E, f)\|_F \quad \text{subject to} \quad (A+E)x = b+f$$

- Classical Algorithm Golub Reinsch Van-Loan

$$\text{Solve } [\hat{A}|\hat{b}] \begin{bmatrix} x_{TLS} \\ -1 \end{bmatrix} = 0, \ \hat{A} = A + E, \ \hat{b} = b + f.$$

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- ▶ Direct Compute the SVD and solve.

Rayleigh Quotient Formulation for TLS

- An Iterative Approach:

$$x_{TLS} = \mathrm{argmin}_x \phi(x) = \mathrm{argmin}_x \frac{\|Ax - b\|^2}{1 + \|x\|^2},$$

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- TLS minimizes the sum of squared normalized residuals.

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- Björck, Hesternes and Matstoms(BHM), 2000 Eigenvalue equation for TLS

$$\begin{pmatrix} A^TA & A^Tb \\ b^TA & b^Tb \end{pmatrix} \begin{pmatrix} x \\ -1 \end{pmatrix} = \sigma^2 \begin{pmatrix} x \\ -1 \end{pmatrix}$$

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- Use Rayleigh quotient iteration to find the minimal eigenvalue.
- Solve *shifted normal equations* by Preconditioned Conjugate Gradients each iteration.

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Reformulation with Lagrange Multiplier If the constraint is active the solution x^* satisfies *normal equations*

$$(A^TA + \lambda_I I + \lambda_L L^TL)x^* = A^Tb, \; (x^*)^T L^T L x^* - \delta^2 = 0,$$

$$\lambda_I = -\frac{\|Ax^* - b\|^2}{1 + \|x^*\|^2}, \quad \lambda_L = \mu(1 + \|x^*\|^2),$$

$$\mu = -\frac{1}{\delta^2}\left(\frac{b^T(Ax^* - b)}{1 + \|x^*\|^2} + \frac{\|Ax^* - b\|^2}{(1 + \|x^*\|^2)^2}\right),$$

Golub, Hansen and O'Leary, 1999. Solution technique is parameter dependent: λ_L, λ_I, δ, μ

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$$\min_x \phi(x) \quad \text{subject to } \|Lx\| \leq \delta.$$

- Augmented Lagrangian

$$\mathcal{L}(x, \mu) = \phi(x) + \mu(\|Lx\|^2 - \delta^2).$$

Eigenvalue Problem RTLS: Renaut & Guo (SIAM 2004)

$$B(x^*)\begin{pmatrix} x^* \\ -1 \end{pmatrix} = -\lambda_I \begin{pmatrix} x^* \\ -1 \end{pmatrix},$$

$$B(x^*) = \begin{pmatrix} A^TA + \lambda_L(x^*)L^TL, & A^Tb \\ b^TA, & -\lambda_L(x^*)\gamma + b^Tb \end{pmatrix},$$

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- Seek the minimal eigenpair for B. Note B is not constant.
- Specify constraint $\|Lx^*\|^2 \leq \delta^2$, use $\gamma = \delta^2$ or $\|Lx^*\|^2$

Development

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- Reformulation:

For a constant δ, find a θ such that $g(x_\theta) = 0$.

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Lemma Assuming that $b^T A \neq 0$ and $\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$, then the smallest eigenvalue of $\mathbf{B}(\theta)$ is simple.

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Lemma If $[A, b]$ is a full rank matrix, there exists one and only one positive number, denoted by θ^c, such that $\mathbf{B}(\theta^c)$ is singular, and

(i) the null eigenvalue of $\mathbf{B}(\theta^c)$ is simple
(ii) when $0 \leq \theta < \theta^c$, $\mathbf{B}(\theta)$ is positive definite, and
(iii) when $\theta > \theta^c$, $\mathbf{B}(\theta)$ has only one negative eigenvalue.

Uniqueness

Lemma If $b^T A \neq 0$, $[A, b]$ is full-rank, then solution of $g(x_\theta) = 0$ is unique and

(i) There exists a $\lambda_L^* \in [0, \theta^c]$ which solves $g(x_\theta) = 0$.
(ii) When $\lambda_L \in (0, \lambda_L^*)$, $g(x_{\lambda_L}) > 0$ and $\lambda_L \in (\lambda_L^*, \infty)$, $g(x_{\lambda_L}) < 0$.

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Observe We see from this result that there is an unique solution to our problem and that an algorithm for finding this solution should depend both on finding an update for the Lagrange parameter λ_L and monitoring the sign of $g(x_{\lambda_L})$.

The Update Equation for $\theta = \lambda_L$

$$\begin{aligned} \lambda_L^{(k+1)} &= \lambda_L^{(k)} + \iota^{(k)} \frac{\lambda_L^{(k)}}{\delta^2} g(x_{\lambda_L^{(k)}}), \\ 0 < \iota^{(k)} &\leq 1 \text{ such that } g(x_{\lambda_L^{(k+1)}}) g(x_{\lambda_L^{(0)}}) > 0. \end{aligned}$$

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Observe $B(\lambda_L^{(k)})$ is always positive definite. For $0 < \lambda_L^{(0)} < \theta^c$ iteration is monotically increasing or decreasing dependent on $\lambda_L^{(0)} >< \lambda_L^*$.

EXACT RTLS: Alternating Iteration on λ_L and x.

Algorithm

Given δ, $\lambda_L^{(0)} > 0$, calculate eigenpair $(\varrho_{n+1}^{(0)}, x^{(0)})$. Set $k = 0$. Update $\lambda_L^{(k)}$ and $x^{(k)}$ until convergence.

1. While not converged **Do** $\iota^{(k)} = 1$

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2. **End Do.** $x_{RTLS} = x^{(k)}$.

Inner Iteration Solve I

- Find eigenvector $y^{(k,j+1)} = ((x^{(k,j+1)})^T, -1)^T$ such that

$$\begin{aligned} \mathbf{B}(\lambda_L^{(k)}) y^{(k,j+1)} &= \beta_{(k,j)} y^{(k,j)}, \\ \mathbf{B}(\lambda_L^{(k)}) &= \begin{pmatrix} J^{(k,j)} & A^T b \\ b^T A & \eta_{(k,j)} \end{pmatrix}, \end{aligned}$$

$$J^{(k,j)} = A^T A + \lambda_L^{(k)} L^T L \qquad \eta_{(k,j)} = b^T b - \lambda_L^{(k)} \delta^2,$$

Inner Iteration Solve II

- Apply Block Gaussian Elimination:

$$\begin{pmatrix} J^{(j)} & A^T b \\ 0 & \tau_j \end{pmatrix} \begin{pmatrix} x^{(j+1)} \\ -1 \end{pmatrix} = \beta_j \begin{pmatrix} x^{(j)} \\ -(z^{(j)})^T x^{(j)} - 1 \end{pmatrix},$$

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$$\tau_j = \eta_j - b^T A z^{(j)} \quad x^{(j+1)} = z^{(j)} + \beta_j u^{(j)} \quad \beta_j = \tau_j / ((z^{(j)})^T x^{(j)} + 1).$$

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- $z^{(j)}$ and $u^{(j)}$ solve $J^{(j)} z^{(j)} = A^T b$, $J^{(j)} u^{(j)} = x^{(j)}$.

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- **Do not shift** For inexact update we do not use the shift because the system matrix $\mathbf{B}$ is parameter dependent and it makes no practical sense to force convergence with the shift.
- **Choice of γ:** The theory is developed for $\gamma = \delta^2$ but the algorithm can use $\gamma = \|Lx^{k,j}\|^2$. If blow up does not occur, the algorithm converges more quickly.

Computational Considerations: Generalized SVD

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$$A = U \begin{pmatrix} \Sigma & 0 \\ 0 & I_{n-p} \end{pmatrix} X^{-1}, \;\; L = V \begin{pmatrix} M & 0 \end{pmatrix} X^{-1}.$$

U, V, $m \times n$ and $p \times p$, resp., orthonormal. X, $n \times n$ nonsingular.Σ, M diag., $p \times p$, entries σ_i μ_i, resp. Then

$$\left[\begin{pmatrix} \Sigma^2 & 0 \\ 0 & I_{n-p} \end{pmatrix} + \lambda_L \begin{pmatrix} M^2 & 0 \\ 0 & 0 \end{pmatrix} \right] X^{-1}w = X^Tf.$$

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- Efficient Direct solution can be found efficiently $8n^2$ flops. Solve triangular systems for each λ_L.

Inverse Problems

Total Least Squares Methods

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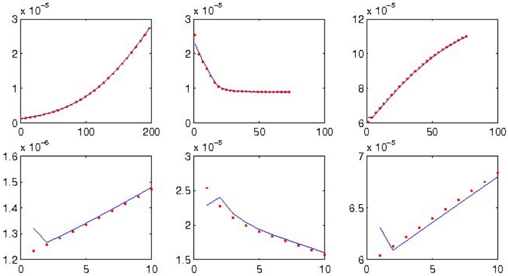
Experiments: Hansen's Regularization Toolbox

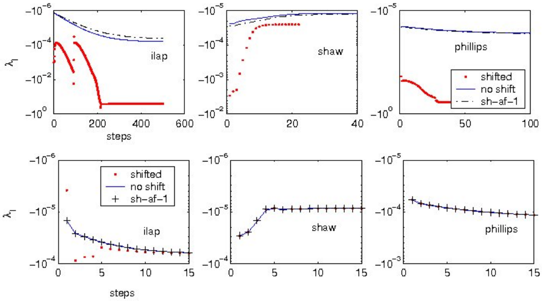
- *ilaplace, phillips* and *shaw* -all discretizations of continuous ill-posed Fredholm integral type constructed by quadrature.
- Generate A and x^*, calculate $b = Ax^*$ exactly.
- Scale $\|A\|_F = \|b\|_2 = 1$.
- Add noise 5% Gaussian to b and A.
- L approxs first derivative, $(n-1) \times n$.
- Tolerance $\tau = 10^{-4}$.
- Estimated solution x_{est}. Relative error with respect to x^*.
- Number of system solves K.

Inexact and Exact Algorithms: convergence for $-\lambda_l^{(k)}$



The dotted and dashed lines show convergence for exact and inexact algorithms, resp.. The first row shows the whole convergence history while the second row shows the first 10 steps. Left to right *ilaplace*, *shaw* and *phillips* resp..

Inclusion of Shift: convergence history of $-\lambda_I$

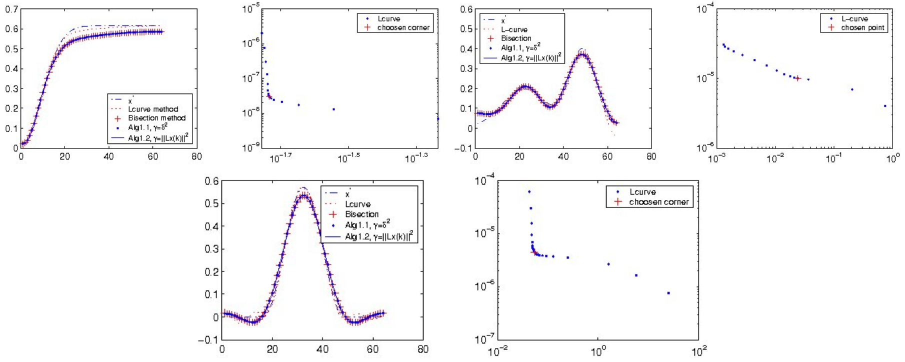


Using $\gamma = \delta^2$ and $\gamma = \|Lx^{k,j}\|^2$. top and bottom, resp.

shifted, no shift, or shift after first step.

ilaplace, *shaw* and *phillips* resp..

Comparison for γ: δ^2 or $\|Lx^{(k,j)}\|^2$



On top *ilaplace*, and *phillips*. Below *shaw*. Solutions are indicated on the left, and the L-curve on the right.

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Regularized Total Least Squares

Numerical experiments have been presented which verify the theory

- The algorithm provides an efficient and practical approach for the solution of the RTLS problem in which a good estimate of the physical parameter is provided.

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- If blow up occurs bisection search may yield a better solution satisfying the constraint condition.
- If no constraint information is provided, the L-curve technique can be successfully employed.
- Algorithm performs better than QEP for all of our tests.

Related Work

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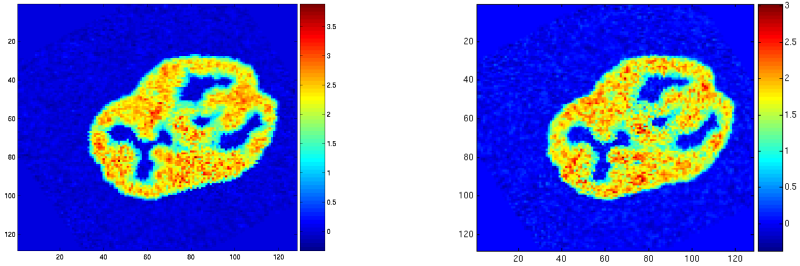
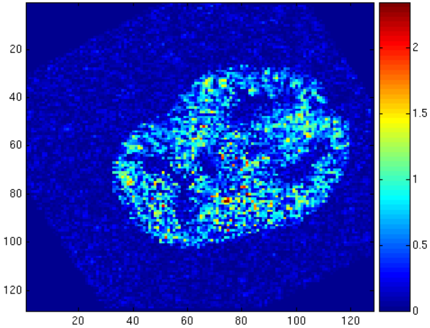
  - Total Variation TLS
  - Large scale implementation
  - Multiple Right Hand Sides.

Removal of Noise from Difference Images for Longitudinal Studies



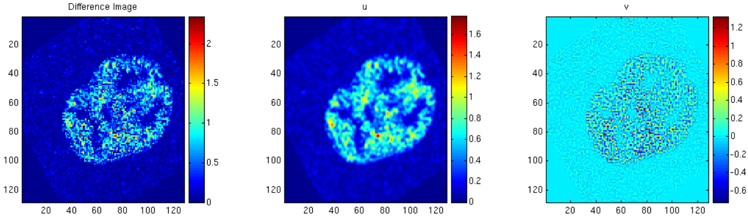
- **Application:** Two PET scans of the same patient at different times
- **Question:** Are there any anatomical or functional changes?

Difference Image after Alignment by Maximization of Mutual Information

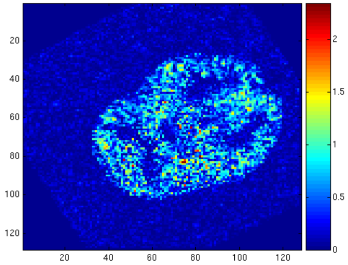


- Scans from different days have to be aligned
- Noise and artifacts change from scan to scan.
- Small changes are hard to locate in the difference image

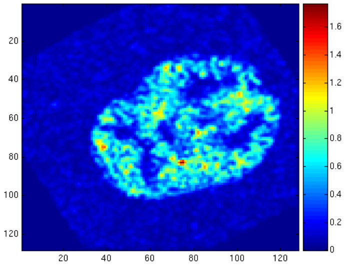
Decomposed Difference Image: wavelets



Difference Image and u Part

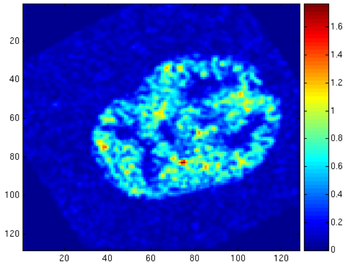


Difference Image

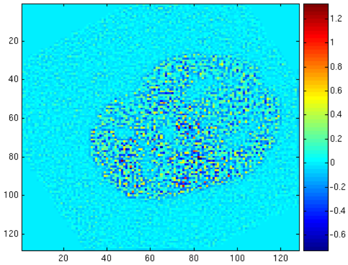


u Part

u and v Part



u Part



v Part

THANKYOU

Any Questions